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Comparisons of Wilks' and Monte Carlo Methods in Response to the 10CFR50.46(c) Proposed Rulemaking

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ABSTRACT

The Nuclear Regulatory Commission (NRC) is proposing a new rulemaking on emergency core system/loss-of-coolant accident (LOCA) performance analysis. In the proposed rulemaking, designated as 10CFR50.46(c), the US NRC put forward an equivalent cladding oxidation criterion as a function of cladding pre-transient hydrogen content. The proposed rulemaking imposes more restrictive and burnup-dependent cladding embrittlement criteria; consequently nearly all the fuel rods in a reactor core need to be analyzed under LOCA conditions to demonstrate compliance to the safety limits. New analysis methods are required to provide a thorough characterization of the reactor core in order to identify the locations of the limiting rods as well as to quantify the safety margins under LOCA conditions. With the new analysis method presented in this work, the limiting transient case and the limiting rods can be easily identified to quantify the safety margins in response to the proposed new rulemaking. In this work, the best-estimate plus uncertainty (BEPU) analysis capability for large break LOCA with the new cladding embrittlement criteria using the RELAP5-3D code is established and demonstrated with a reduced set of uncertainty parameters. Both the direct Monte Carlo method and the Wilks' nonparametric statistical method can be used to perform uncertainty quantification. Wilks' method has become the de-facto industry standard to perform uncertainty quantification in BEPU LOCA analyses. Despite its widespread adoption by the industry, the use of small sample sizes to infer statement of compliance to the existing 10CFR50.46 rule, has been a major cause of unrealized operational margin in today's BEPU methods. Moreover the debate on the proper interpretation of the Wilks' theorem in the context of safety analyses is not fully resolved yet, even more than two decades after its introduction in the frame of safety analyses in the nuclear industry. This represents both a regulatory and application risk in rolling out new methods. With the 10CFR50.46(c) proposed rulemaking, the deficiencies of the Wilks' approach are further exacerbated. The direct Monte Carlo approach offers a robust alternative to perform uncertainty quantification within the context of BEPU analyses. In this work, the Monte Carlo method is compared with the Wilks' method in response to the NRC 10CFR50.46(c) proposed rulemaking.

KEYWORDS

LOCA, BEPU, 10CFR50.46(c), Wilks's nonparametric statistical method, Monte Carlo

1. INTRODUCTION

The current emergency core cooling system (ECCS) acceptance criteria for loss-of-coolant accidents (LOCA) in light-water reactors (LWRs) are described in 10CFR50.46. Two of the five criteria specify that the calculated peak cladding temperature (PCT) and maximum cladding oxidation shall not exceed 2200°F (1478K) and 17% equivalent cladding reacted (ECR), respectively [1]. Ever since the establishment of these cladding embrittlement criteria, more extensive research and experiments have been conducted which resulted in an increased understanding of fuel and clad behavior under both normal operating conditions and LOCA transient conditions. The new studies indicated that the current regulatory acceptance criteria may be non-conservative for high burnup fuel. The Nuclear

Regulatory Commission (NRC) is considering a rulemaking change that would revise the requirements in 10CFR50.46. In the proposed new rulemaking, designated as 10CFR50.46(c), the NRC proposed a fuel performance-based ECR criterion as a function of cladding hydrogen content before the accident (pre-transient), to include the effects of fuel burnup on cladding performance [2]. The pre-transient cladding hydrogen content, in turn, is a function of the fuel burnup and cladding materials. A characteristic of the proposed new rulemaking, as illustrated in Figure 1, imposes more restrictive and fuel rod-dependent cladding embrittlement criteria. Consequently fuel cladding performance and ECCS performance need to be considered in a stronger coupled way in LOCA analyses.

The aforementioned discussions indicate that a more detailed modeling of the reactor core is required in LOCA analyses in order to provide a through characterization of the core. In this study, we will present the methods and results from the demonstration of applying the best-estimate plus uncertainty (BEPU) methodology using the RELAP5-3D code to a large break LOCA (LBLOCA) analysis in response to the proposed new rules in 10CFR50.46(c). The results from the widely used Wilks nonparametric statistical method will be compared with the direct Monte Carlo method.

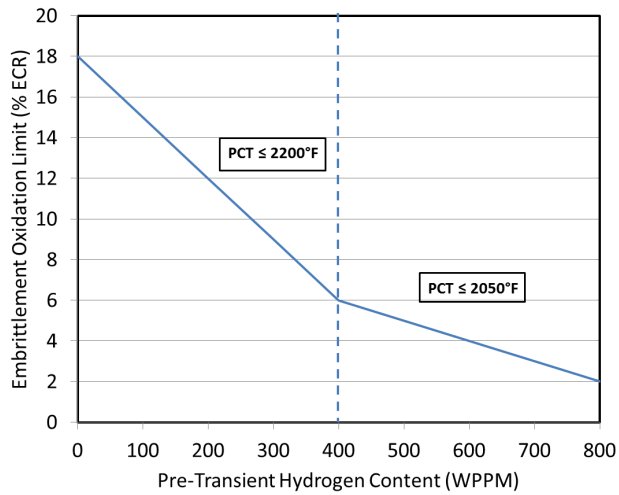

Fig. 1 Analytical Generic Limit Proposed by the NRC for Existing Fuel, ECR & PCT versus Hydrogen [2].

2. BRIEF REVIEW OF BEPU METHODOLOGY IN LBLOCA ANALYSIS

Best estimate plus uncertainty (BEPU) methodology has become the de-facto industry standard to demonstrate compliance under the existing rule specified in 10CFR50.46. Generally, there are two types of methods that can be used to perform uncertainty quantification within the context of BEPU, direct Monte Carlo method and Wilks' method. Direct Monte Carlo method simply samples the input distributions a large number times (N) and then uses computer codes to generate N output files which are then used to generate the distribution of safety metrics or figure of merits (FOM). The direct Monte Carlo method requires formidable computing resources if directly using system analysis codes and is considered to be impractical for industrial applications in the past. Lately with the ever increasing computing power, this approach has the potential to be widely adopted by the industry. On the other hand, the Wilks's method is widely used with the current industry practice to perform uncertainty quantification. Wilks' method [3], originally proposed by S.S. Wilks in 1941 for use in manufacturing processes, is a nonparametric statistical analysis method which provides a bounding value of the samples with a given confidence level. This method can be referred to as "distribution-free" method. Like the direct Monte Carlo method, the Wilks' method randomly samples all the uncertainty parameters in the space defined by the uncertainty ranges and all the uncertainties are combined. However it only uses small number of samples to aggregate the effect of the uncertainty parameters to quantify the total uncertainty in the LOCA analysis. This method decouples

the number of uncertain parameters from the number of required calculations in order to perform uncertainty quantification analysis. It has the advantage of using a relatively small number of samples of LOCA transient calculations to obtain the limiting transient case as well as the 95/95 (95% probability with 95% confidence level) upper tolerance limits of the safety metrics. A set of equations was derived through which the number of required data samples can be solved for a desired tolerance limit and confidence level. The equation for one-sided tolerance limits is given as

$$1 - \beta^N > \gamma \tag{1}$$

where β is the desired probability of coverage, γ is the confidence level, and N is the minimum number of required data samples. If we are interested in finding out the minimum number of data samples for 95/95 upper tolerance limits, substituting β=0.95 and γ=0.95 into Eq. (1) and N is found to be 59. Eq. (1) is applicable to situations where only one outcome, e.g. PCT, is measured from the sample. However if more than one outcome is measured from the sample the sample size needs to be extended beyond 59 runs. The number of runs can be found by solving the following equation for N [4]:

$$\beta = \sum_{j=0}^{N-p} \frac{N!}{(N-j)!j!} \gamma^j (1-\gamma)^{N-j} \tag{2}$$

where p is the number of outcomes considered and N is number of required sample size. With the proposed new rule in 10CFR50.46(c), at a minimum two safety metrics, PCT and ECR, have to be considered to demonstrate compliance to the safety limits acceptance criteria. If we substitute γ=0.95, β=0.95 and p=2 into the Eq. (2), N is found equal to 93.

In the current practice of LOCA analysis with 10CFR 50.46 rules, the limiting fuel rod in the limiting transient case can be easily identified with the safety metric being defined as the PCT and the limiting rod as the fuel rod with the highest PCT, which is normally the highest power rod (hot rod). The reactor core modeling in a large break LOCA analysis normally uses a simplified approach with the core flow represented by a hot channel and an average channel. The hot channel represents the flow channel adjacent to the highest power rod and the average flow channel represents the remaining flow in the core. The fuel and clad temperature distributions and clad oxidation rates within the hot rod are calculated by building a heat structure for the rod and attaching it to the hot channel. Average heat structures are built for the remaining fuel rods in the core and attached to the average flow channel such that the fuel and clad temperature distributions and clad oxidation rates can be calculated for the average rods. Conversely, with the proposed new rulemaking in 10CFR50.46(c), both the PCT and ECR safety acceptance criteria are functions of the pre-transient hydrogen content in the clad. The limiting rods may not be the hot rod (highest power rod) and could even move from one fuel rod location to another depending on fuel burnup and other conditions in an operating cycle. Therefore, new safety metrics (figures of merits) have to be defined in compliance with 10CFR50.46(c) and all the fuel rods have to be considered in LOCA analyses in order to identify the limiting rods. Since both PCT and ECR limits are burnup-dependent, the new safety metrics would need to synthesize PCT and ECR with fuel rod dependent cladding pre-transient hydrogen content. As a result, the safety metrics are defined as the ratios of the calculated PCT over PCT limits for each fuel rod, as well as the ratios of the calculated ECR over ECR limits for each fuel rod and are expressed in the following:

$$PCTR = \frac{PCT^{Calculated}}{PCT^{Limit}} \tag{3}$$

$$ECRR = \frac{ECR^{Calculated}}{ECR^{Limit}} \tag{4}$$

If we define $PCTR_{max}$ and $ECRR_{max}$ as the maximum value of PCTR and the maximum value of ECRR, respectively, the acceptance criteria for the safety metrics are the following:

1) $PCTR_{max} < 1.0$

or

2) $ECRR_{max} < 1.0$

Using the above criteria, the limiting fuel rods can be identified as the fuel rods with the maximum PCTR value ($PCTR_{max}$) or the maximum ECRR value ($ECRR_{max}$) during LOCA transients. Using Wilks' theorem, compliance can be demonstrated by ranking the PCTR and ECRR obtained from the simulations in the 93 samples. The highest ranked set of PCTR and ECRR from the 93 samples can be chosen as the limiting cases to represent the 95/95 estimates of the upper tolerance of the chosen safety metrics from a small sample.

Despite the widespread adoption of the Wilks' method by the industry, the use of small sample sizes to infer statement of compliance to the 10CFR50.46 rule has been a major cause of unrealized operational margin in today's BEPU methodology. With a small sample size, the Wilks' method has the risk of under-prediction or over-prediction of figures-of-merit. Additionally, reliable sensitivity analysis results are not attainable with a small sample size to gain the insights in what's truly limiting in the design in order to assess the impact of design changes. Moreover, the debate on the proper interpretation of the Wilks' theorem in the context of safety analyses is not fully resolved yet more than two decades after its introduction in the nuclear industry. This represents both a regulatory and operational risk in rolling out new methods. Due to the added complexity with the 10CFR50.46(c) proposed rulemaking, the deficiencies of the Wilks' approach are further exacerbated. The direct Monte Carlo approach offers a robust alternative to perform uncertainty quantification within the context of BEPU analyses. It should be pointed out that, using the direct Monte Carlo method, very large sample sizes may be needed to reduce the confidence interval on the estimate of safety metrics to the desired magnitude. However with the direct Monte Carlo simulations, sensitivity analyses can be performed such that the impact and significance of input parameter changes can be assessed with high confidence. In this work, the Monte Carlo method is compared with the Wilks' method in response to the NRC's 10CFR50.46(c) proposed rulemaking.

3. RELAP5-3D MODEL DESCRIPTION FOR A TYPICAL PWR

A typical four-loop pressurized water reactor (PWR) with 3411 MW rated thermal power has been selected for analysis with RELAP5-3D. RELAP5-3D is a reactor system safety analysis code developed at Idaho National Laboratory [5]. The accident scenario selected is a LBLOCA with a double-ended guillotine break in a cold leg. The nodalization diagram of the RELAP5-3D model for the typical PWR is shown in Figure 2.

The reactor core has 193 assemblies with three batches of fuel loading – the fresh fuel, once-burnt fuel and twice-burnt fuel. An equilibrium cycle was achieved for this core design [6] and the results were fed into the RELAP5-3D model. The details of the core physics analysis tools and core design parameters can be found in [6].

The reactor core modeling in RELAP5-3D used different homogenization approaches for thermal fluid dynamics calculations than for the heat conduction and clad oxidation calculations in the fuel rods. A multiple channel approach was used for the thermal fluid dynamics calculation, as illustrated in Figure 3. Specifically, the assemblies in the core were grouped into various regions based on their burnup history. The assemblies with fresh fuel, once-burnt fuel and twice-burnt fuel were grouped together respectively. Two flow channels – one average channel and one hot channel – were built to represent each group of assemblies. Hence there are a total of six flow channels in this study. The flow channels are connected in the lateral direction to allow crossflow to be calculated. Crossflow is modeled at each axial elevation in the core between the three average core channels. It is also modeled at each axial elevation between the hot channels and the adjacent average channels. This allows flow to be redistributed around a blockage caused by cladding ballooning or rupture. The crossflow area is based on the minimum gap between the fuel rods along one side of a fuel assembly and the number of fuel assembly sides at the interface between the three average core channels; for example, for the hot

assembly in each region, there are four sides at the interface. Loss coefficients are approximated based on flow across in-line and staggered rows of tubes, with the average distance of travel estimated to be about half an assembly width.

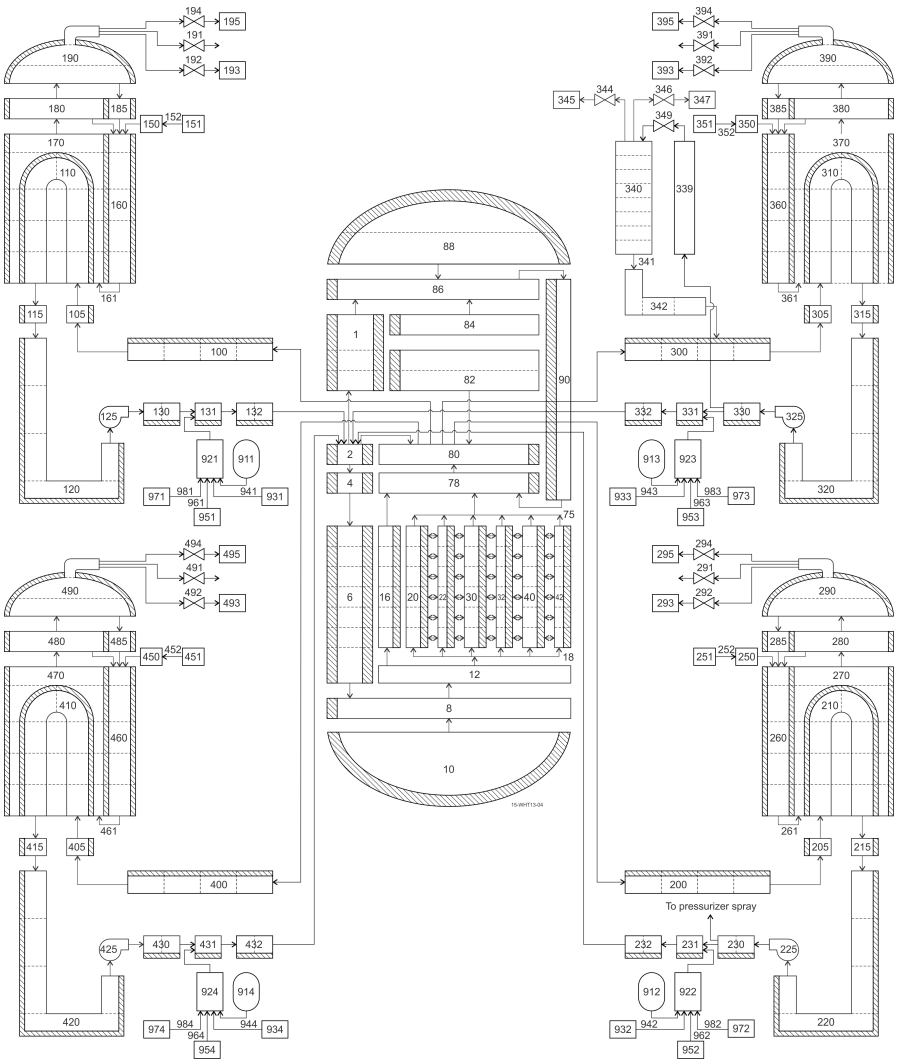

Fig. 2 RELAP5-3D Nodalization of a Typical Four-Loop PWR.

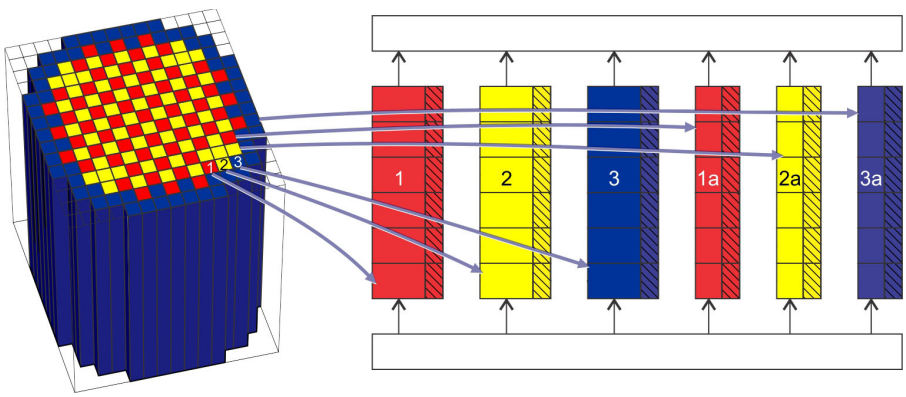

Fig. 3 Schematic Illustration of the Mapping Between the Core Design Analysis and the RELAP5-3D Analysis Core Model for a Typical Four-Loop PWR.

For heat conduction and clad oxidation calculations, it is computationally prohibitive to consider all the fuel rods in the reactor core. Instead a homogenization technique is used to reduce the number of fuel rods to be simulated. Two sets of heat structures were used for each assembly – one set represents the highest power rod or the hot rod in the assembly and the other set represents the average of the remaining fuel rods in the assembly. This is a reasonable approximation given that the fuel rod burnup normally does not vary too much within a PWR assembly and the hot rod in an assembly would be the limiting rod for that assembly.

As a result, heat structures for the highest power assembly (hot assembly) and its hot rod in each group of assemblies were built and attached to the hot channel, as shown schematically in Figure 4, such that the PCT and ECR in the average rods and hot rod can be calculated. Analogously, the heat structures for the other assemblies and their respective hot rods were built and connected to the average channel, as shown in Figure 5, such that the PCT and ECR can be calculated for the average rods and hot rod in each assembly. Therefore, there are a total of 386 sets of heat structures for the fuel in this study (193 for assemblies plus 193 for hot rods). It is noted that the hot rod power has been subtracted from each assembly to yield the correct power for the average fuel rods in each assembly such that the reactor total power is conserved.

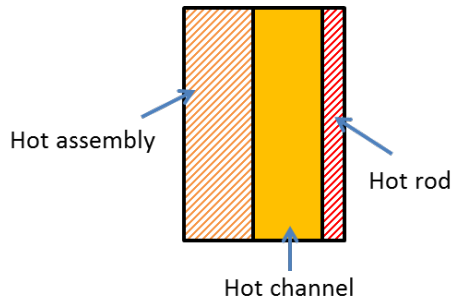

Fig. 4 Schematic Illustration of the Heat Structure Mapping for the Hot Assembly and Its Hot Rod With the Hot Channel (One for Each Group of Assemblies).

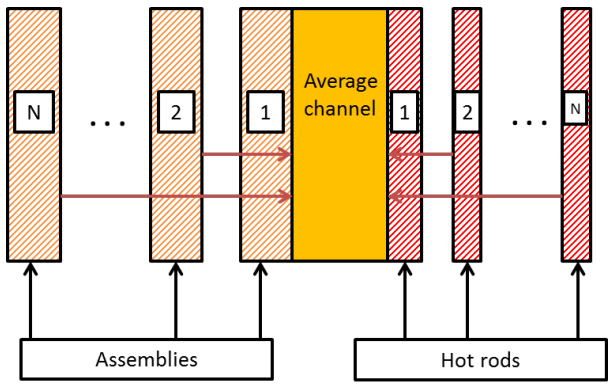

Fig. 5 Schematic Illustration of the Heat Structure Mapping for Average Assemblies and Their Respective Hot Rods with the Average Flow Channel.

In order to perform BEPU analyses, the important phenomena affecting the progression of the LBLOCA accident are first determined by the phenomena identification and ranking table (PIRT) process. A large number of studies have been done previously to identify the important phenomena. A PIRT analysis has been conducted in this work with input from FPoliSolutions LLC [6]. For demonstration purposes, a reduced set of parameters with high importance to LBLOCA has been selected and is shown in Table 1.

Table 1. Distribution of parameter uncertainties

Parameter	PDF type	Min	Max	Comments
Reactor thermal power	Normal	0.98	1.02	Multiplier
Reactor decay heat power multiplier	Normal	0.94	1.06	Multiplier
Accumulator pressure	Normal	-0.9	1.1	Multiplier
Accumulator liquid volume (m^3)	Uniform	-0.23	0.23	Additive
Accumulator temperature (K)	Uniform	-11.1	16.7	Additive
Subcooled multiplier for critical flow	Uniform	0.8	1.2	Multiplier
Two-phase multiplier for critical flow	Uniform	0.8	1.2	Multiplier
Superheated vapor multiplier for critical flow	Uniform	0.8	1.2	Multiplier
Fuel thermal conductivity	Normal	0.93	1.07	Multiplier
Average core coolant temperature (K)	Normal	-3.3	3.3	Additive
Film boiling heat transfer coefficient	Uniform	0.7	1.3	Multiplier

4. COMPARISONS OF WILKS'S AND MONTE CARLO METHOD

A LOCA analysis toolkit has been developed using the Python programming language. The LOCA toolkit automatically samples each uncertain parameter shown in Table 1 from its distribution. For a uniform distribution, the minimum and maximum values are the boundaries of the sampling. For a normal distribution, the sampling boundaries are truncated at the minimum and maximum values, which is effectively a truncated normal distribution. No dependencies between parameters are considered in the sampling. The LOCA toolkit then modifies the RELAP5-3D input files according to the perturbed values. It automatically drives the desired number of RELAP5-3D runs on Idaho National Laboratory's high performance computers (HPC). The toolkit also performs the postprocessing of the RELAP5-3D output files and presents the $PCTR_{max}$ and $ECRR_{max}$ values for each RELAP5-3D output file. Figure 6 illustrates the data flow process within the BEPU analysis toolkit.

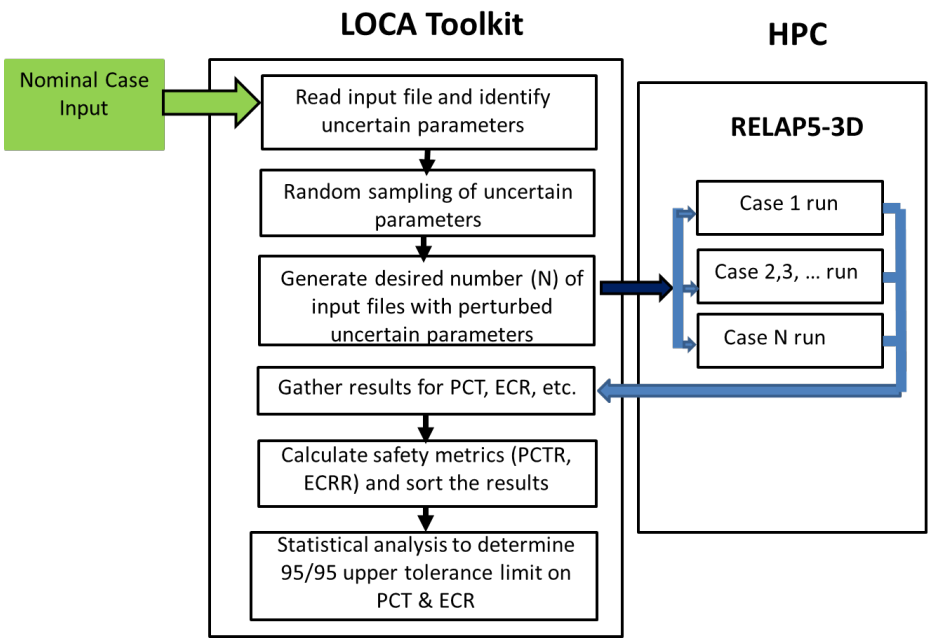

Fig. 6 Diagram of Data Flow Process with the LOCA Toolkit.

Using the LOCA toolkit, the input parameter uncertainties were propagated via Monte Carlo sampling and direct Monte Carlo simulations have been carried. We chose to have 1023 RELAP5-3D input files generated and run at BOC, 300 and 500 days respectively. These three cycle exposure points were selected to represent the plant conditions at the beginning of cycle, middle of the cycle and the end of

the cycle. Consequently, a total of 3069 large break LOCA cases have been run with RELAP5-3D on Idaho National Laboratory's (INL's) high performance computers. The $PCTR_{max}$ and $ECRR_{max}$ values from each RELAP5-3D output file are obtained and then sorted by the LOCA toolkit among the 1023 runs respectively at the three selected cycle exposure points. For illustrative purpose, the probability distribution function (PDF) and cumulative distribution functions (CDF) for PCTR and ECRR at 300 days are shown in Figures 7 and 8 respectively. It can be seen that several cases violated the PCTR limits but met the ECRR limits.

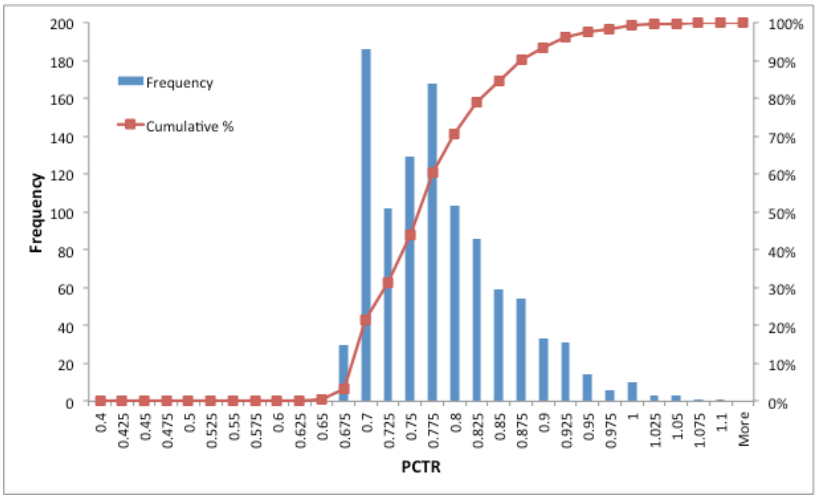

Fig. 7 PDF and CDF for PCTR at 300 Days.

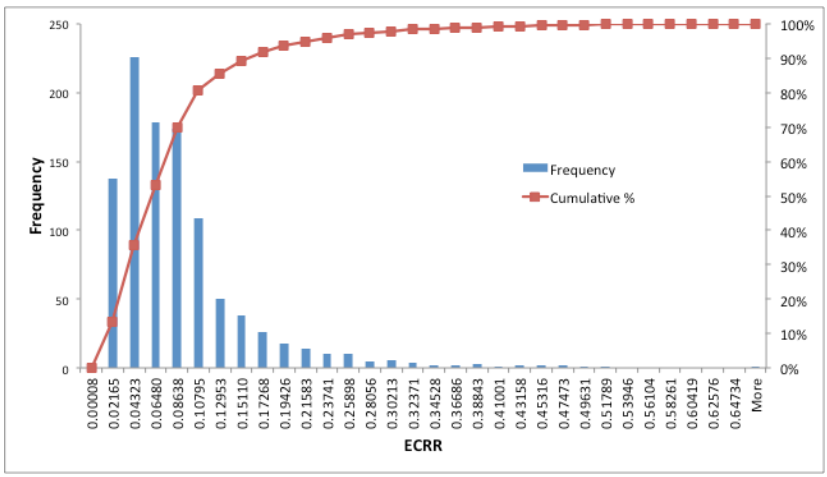

Fig. 8 PDF and CDF for ECRR at 300 Days.

From the cumulative distribution functions of PCTR and ECRR, the 95 percentile values of PCTR and ECRR, as well as of their corresponding PCT and ECR values, are obtained and their associated 95% confidence interval are subsequently calculated to construct the common "95/95" estimators of the upper tolerance limits for PCT and ECR. The 95/95 estimators are compared to the proposed 10CFR50.46(c) rule to demonstrate compliance. According to Ref. [6], The 95% values with 95% confidence interval can be expressed as:

$$Y_{95/95} = \mu_{95\%} \pm 2 * SE_M \tag{5}$$

Where $\mu_{95\%}$ is the 95 percentile values of PCT or ECR and SE_M is the standard error of the sample mean value. Table 2 shows the 95 percentile value and $2 * SE_M$ from the Monte Carlo simulations at BOC, 300 days and 500 days. Figures 9 and 10 show the 95% PCT and ECR values with 95% confidence intervals respectively at BOC, 300 days and 500 days from the Monte Carlo simulations.

Table 2. Summary of Monte Carlo Simulation Results

	PCT (K)		ECR (%)	
	$\mu_{95\%}$	$2 * SE_M$	$\mu_{95\%}$	$2 * SE_M$
BOC	1150.08	4.43	0.97	0.02
300 Days	1350.29	6.99	3.41	0.07
500 Days	1215.99	4.94	2.32	0.06

The Monte Carlo sampling 95/95 estimator is then compared to Wilks based 95/95 upper tolerance estimators. A single Monte Carlo sampling sequence is divided up into *N* Wilks groups depending on the required sample size for a particular Wilks based estimator. Since the PCTR and ECRR are the figures of merit considered in this analysis, based on Wilks theorem the required number of samples for Wilks based estimator is 93 from Eq. (2). The 1023 Monte Carlo samples at BOC, 300 days and 500 days, respectively, are randomly divided into 11 groups of Wilks based estimators. Each Wilks based estimator consists of 93 RELAP5-3D LBLOCA runs. The PCTR and ECRR from the each group of the 93 runs are extracted and sorted from maximum to minimum. From Wilks theorem, rank 1 in each of the 93 samples is considered to be the 95/95 upper tolerance limit. The corresponding values of PCT and ECR from the rank 1 of PCTR and ECRR are obtained. The mean value and standard deviation of PCT and ECR from the 11 Wilks based estimators are then calculated to construct a distribution of the Wilks based estimators. Table 3 shows the mean estimate of the Wilks based estimators with one standard deviation. Figures 11 and 12 show the mean estimate of the Wilks based estimators for PCT and ECR respectively with the error bar extremes indicating $\pm$ one standard deviation (1σ) around this mean.

Using the data presented in Tables 2 and 3 and Figures 9 - 12, the distribution of the Wilks based 95/95 estimators can then be compared to the Monte Carlo sampling 95/95 estimator. The comparison shows that the Wilks based method can have considerable conservative bias relative to the true 95 percentile upper tolerance limits. This bias could represent the margin loss for a plant owner. Additionally, the Wilks based method has substantial variability. In contrast, the Monte Carlo method provides remedies to both situations. Large sample sizes used by the direct Monte Carlo method provide more accurate estimates to the true 95% upper tolerance limit and the variability is significantly reduced. However, it is noted that there are still several issues to be resolved with using the direct Monte Carlo method, particularly on how to determine the adequate number of calculations to sufficiently represent the output distribution and extract knowledge about the importance and effect of each contributors. To simply put, how do we know if the Monte Carlo simulations converged? Another issue that could be an obstacle for wide application of the Monte Carlo simulations is that, like any existing thermal hydraulic analysis codes, RELAP5-3D has noticeable rate of early crashes when massive simulations are performed. We are able to resolve such issue in this work by adjusting the time step sizes for the crashed cases to make them run to completion. However, for other applications such risk-informed safety margin characterization (RISMC) type of analyses which combine probabilistic and deterministic analyses together to quantify "probabilistic safety margin" [7], much larger number of cases (on the order of tens of thousands to millions) have to be run. A probabilistic safety margin (or quantitative safety margin) is a numerical value quantifying the probability that a key safety metric, such as PCT or ECR, will be exceeded under specified accident scenario conditions. Early crashes could become an insurmountable unavoidable obstacle for such situations. These warrant further studies in the future work.

Table 3. Summary of Wilks based 95/95 estimators for PCT and ECR

	PCT (K)		ECR (%)	
	Mean	Standard Deviation	Mean	Standard Deviation
BOC	1242.67	33.86	2.33	0.68
300 Days	1491.52	71.89	6.45	1.81
500 Days	1378.34	86.50	5.10	1.58

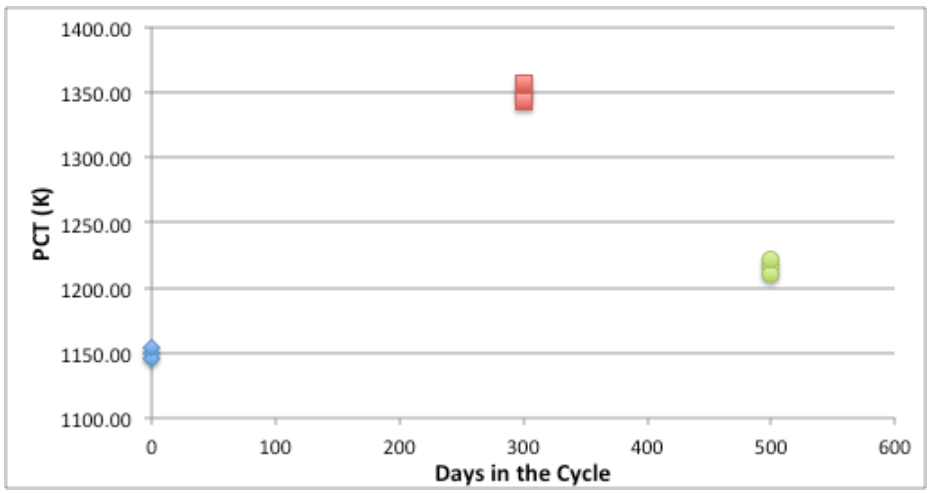

Fig. 9 95% PCT Value with 95% Confidence Interval from Monte Carlo Simulations.

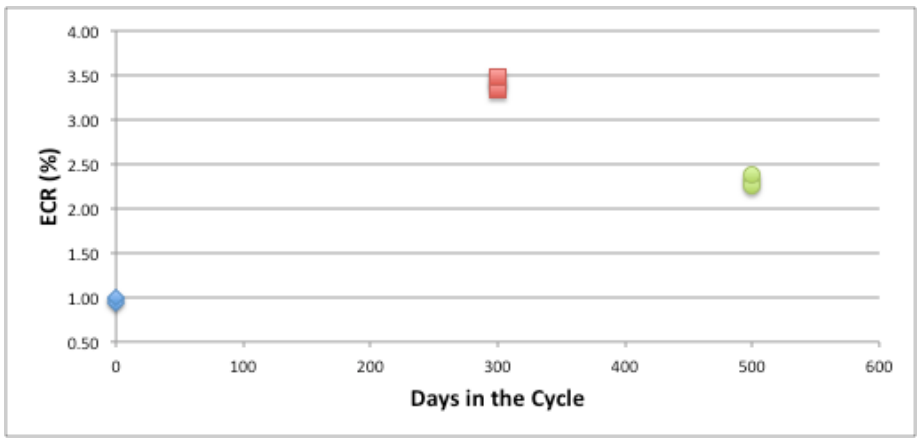

Fig. 10 95% ECR Value with 95% Confidence Interval from Monte Carlo Simulations.

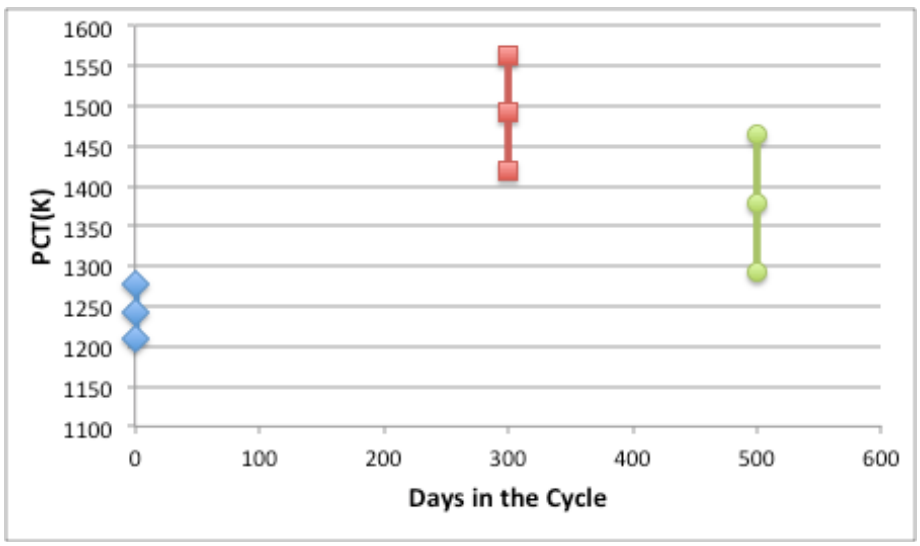

Fig. 11 Wilks Based Mean 95/95 PCT Value $\pm 1\sigma$.

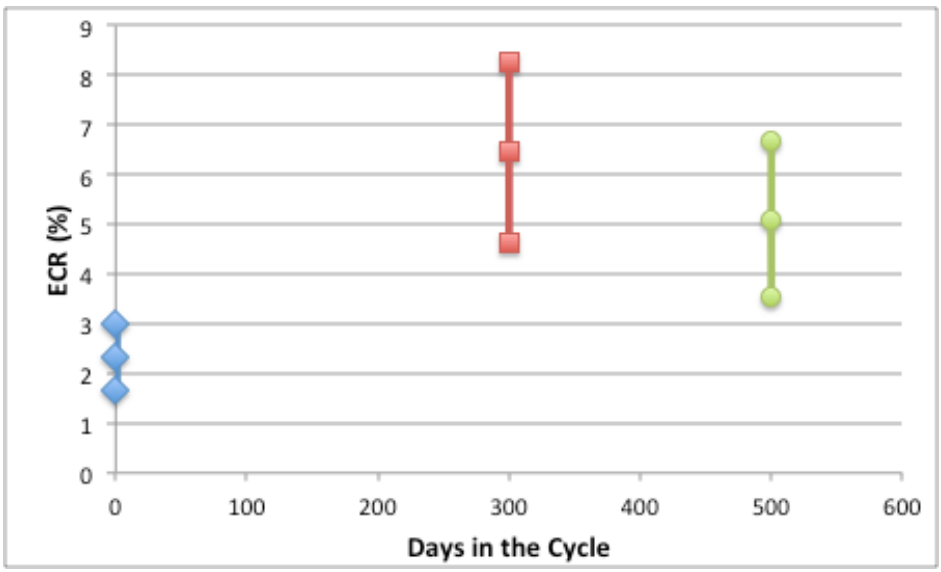

Fig. 12 Wilks Based Mean 95/95 ECR Value $\pm 1\sigma$.

4. CONCLUSIONS AND FUTURE WORK

In this paper, a new analysis approach has been proposed in response to the NRC proposed 10CFR50.46(c) new rulemaking. Both the direct Monte Carlo method and the Wilks nonparametric statistical method have been carried out to perform uncertainty quantification. The comparison results indicate that the commonly used Wilks based method has substantial conservatism and large variability. Direct Monte Carlo method would provide more accurate estimates to the true 95% upper tolerance limits with much reduced variability.

It is noted that fuels performance calculations have not been incorporated into the LOCA calculations yet in this work. Once fuels performance calculations are incorporated into the analysis process, more uncertain parameters, such as gap conductance, rod burst, fission gas release, crud, oxidation layer thickness etc., related to fuel rods can be included in the uncertainty quantification analysis. That is left for future work.

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